AFRL-MN-EG-TN-2001-7070

STUDIES OF THE MECHANICS AND COMBUSTION OF ENERGETIC MATERIALS FOR THE DESIGN OF EXPLOSIVE SYSTEMS

D. Scott Stewart
Theoretical and Applied Mechanics
University of Illinois
100 B Talbot Laboratory
104 S. Wright St.
Urbana, IL 61801

CONTRACT NO. F08630-95-1-0004

MAY 2001

FINAL REPORT FOR PERIOD JANUARY 1995 – JANUARY 2000

DISTRIBUTION A: Approved for public release; distribution unlimited

AIR FORCE RESEARCH LABORATORY, MUNITIONS DIRECTORATE

Air Force Materiel Command ■ United States Air Force ■ Eglin Air Force Base

NOTICE

When Government drawings, specifications, or other data are used for any purpose other than in connection with a definitely Government-related procurement, the United States Government incurs no responsibility or any obligation whatsoever. The fact that the Government may have formulated or in any way supplied the said drawings, specifications, or other data, is not to be regarded by implication, or otherwise in any manner construed, as licensing the holder, or any other person or corporation; or as conveying any rights or permission to manufacture, use, or sell any patented invention that may in any way be related thereto.

This technical note is releasable to the National Technical Information Services (NTIS). At NTIS it will be available to the general public, including foreign nations.

Contract Number: F08630-95-1-0004

Contractor: University of Illinois
PI: Dr. D. Scott Stewart

This technical note has been reviewed and is approved for publication.

FOR THE COMMANDER

Paul K Laird

PAUL K. LAIRD
Tech Director, Ordnance Division

KEITH M. ROESSIG, Capt, USAF
Program Manager

KIRK E. HERZOG
Tech Advisor, Damage Mechanisms Branch

Anyone having need for a copy of this report should first contact the Defense Technical Information Center (DTIC) at the address shown below. If you are a registered DTIC User, DTIC can provide you with a copy. Please do not request copies from the Air Force Research Laboratory, Munitions Directorate. Requests for additional copies should be directed to:

Defense Technical Information Center (DTIC)
8725 John J. Kingman Road, Ste 0944
Ft Belvoir, VA 22060-6218

This report is published in the interest of the scientific and technical information exchange. Publication of this report does not constitute approval or disapproval of the ideas or findings

If your address has changed, if you wish to be removed from our mailing list, or if your organization no longer employs the addressee, please notify AFRL/MNMW, Eglin AFB FL 32542-6810, to help us maintain a current mailing list. Do not return copies of this report unless contractual obligations or notice on a specific document requires that it be returned.

REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. AGENCY USE ONLY *(Leave blank)*	2. REPORT DATE	3. REPORT TYPE AND DATES COVERED
	2001 MAY	FINAL JANUARY 1995-JANUARY 2000

4. TITLE AND SUBTITLE

STUDIES OF THE MECHANICS AND COMBUSTION OF ENERGETIC MATERIALS FOR THE DESIGN OF EXPLOSIVE SYSTEMS

5. FUNDING NUMBERS

Contract #: F08630-95-1-0004
JON:25020693 PE:62602F
PR:2502
TA:06
WU:93

6. AUTHOR(S)

DR. D. SCOTT STEWART

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)

UNIVERSITY OF ILLINOIS
THEORETICAL AND APPLIED MECHANICS
100 B TALBOT LABORATORY
104 S. WRIGHT ST.
URBANA, IL 61801

8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)

AIR FORCE RESEARCH LABORATORY/MUNITIONS DIRECTORATE
DAMAGE MECHANICSMS BRANCH
101 W. EGLIN BLVD. STE 135
EGLIN AFB, FL 32542-6810
PROGRAM MANAGER: CAPT KEITH M. ROESSIG (850) 882-9643 EXT. 266

10. SPONSORING/MONITORING AGENCY REPORT NUMBER

AFRL-MN-EG-TN-2001-7070

11. SUPPLEMENTARY NOTES

12a. DISTRIBUTION/AVAILABILITY STATEMENT

DISTRIBUTION A: Approved for public release; distribution unlimited

12b. DISTRIBUTION CODE

(Leave this block blank)

13. ABSTRACT:

This is the final report that summarizes the research activities carried out under the grant F08630-95-1-0004 (for 5 year, period 01/30/95 to 01/29/00), awarded to the University of Illinois (D. Scott Stewart, Principle Investigator) and the Air Force Research Laboratory, Munition Directorate, Eglin AFB. The major research findings are summarized in the Discussion of Research Accomplishments and they describe 1) development of new models for reactive flow and ignition of energetic materials, 2) improved computational ability for reactive flow and ignition problems, 3) the transfer of detonation propagation algorithms to explosive design codes. A bibliography of all the main archival research papers and technical reports are included with their abstracts.

14. SUBJECT TERM

Detonation shock dynamics; DSD; mechanical ignition; reactive flow; shock wave; equation of state; detonation velocity; curvature

15. NUMBER OF PAGES

30

16. PRICE CODE

17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT
UNCLASSIFIED	UNCLASSIFIED	UNCLASSIFIED	UL

Detonation Shock Dynamics, Detonation, Level-Set Methods, Program Burn, Mechanical Ignition of Energetic Materials

Preamble

This program was conducted by the University of Illinois, (UIUC), Urbana IL 61801 (D. Scott Stewart, Principle Investigator) under contract F08630-95-1004 for the Air Force Research Laboratory, Munitions Directorate, Eglin AFB. The most recent AF program manager, at the completion of the grant, was Captain Keith Roessig of AFRL/MN, Warhead Branch. The grant research was carried out during the period 01/30/95 to 01/29/00.

Contents

1 Description of Research Accomplishments

1.1 Overview

The major aims of this grant as described in the original proposal were to 1) develop improved analytical models for multi-dimensional reactive flow and ignition of energetic materials 2) improve computational capability for reactive flow and ignition problems 3) transfer new algorithms to explosive design codes and 4) document advances in the theory and computation of reactive compressible flow relevant to the explosive system design process.

The support given by the AFRL/Munitions Directorate over the past eight years, (from this grant and a previous three-year contract) has enabled dramatic advances in detonation theory and numerics for application to the design of explosive systems. In particular, D. S. Stewart in collaboration with J. B. Bdzil of Los Alamos National Laboratory, have pioneered the theory of Detonation Shock Dynamics (DSD) as documented in numerous archival publications. The DSD method uses theoretical analyses of the reaction zone structure to determine how the lead detonation shock moves. In particular one determines the relation between the normal detonation shock velocity, the shock curvature and other higher derivatives of the shock surface. This analysis then leads to simplified methods to predict the shock motion. The methods also lead to ways to characterize classes of explosives.

The University of Illinois has been the focal point and originator for many of the most recent theoretical and numerical advances. In particular, prototype numerical codes have been written for DSD-characterization of condensed explosives with real material properties and for DSD-wave tracking and burn time calculations. DSD-technology has been installed in major National Laboratory hydrocodes and that activity is ongoing. The scientific predictions of the DSD-theory for explosives have been validated by direct numerical simulation (DNS). New engineering strategies have been developed for explosive design based on this relatively new science. New models based on continuum mechanics have been developed for modeling the ignition of energetic material from its realization as a solid, all the way to a reactive gas. Most if not all current trends in national defense applications that involve insensitive munitions and miniaturization for explosive systems can make effective use of this technology and continuing research developments in this area.

1.2 Chronology of Activities

In what follows below, we give a chronology of research activities and developments that were undertaken. We make reference to the papers and reports that documented this work and in Section 2. one can find abstracts or summaries of those reports, with more details. All of the papers and reports and associated computer codes have been delivered to Eglin engineers throughout the course of the grant. Additional copies of these materials are available on request.

The fall of 94 was effectively the end of our previous contract with the Munitions Directorate. The status of DSD - theory and related computational algorithms had significantly advanced by the work on that contract. A new set of robust numerical methods based on level-sets had been identified for propagating DSD shock wave in three dimensions and prototype codes had been written. The effect of shock acceleration on DSD-theory had been considered for the first time. The numerical capability to work on complex multi-D problems with embedded boundaries had been significantly advanced.

However most if not all the developments in numerics and theory had been carried out for an explosive described by an ideal EOS. Hence the work of this grant focused on theory and numerics for explosive with real properties, described by non-ideal EOS. Also work was carried out to implement DSD-routines and transition them into AF and Department of Department of Energy (DOE) hydrocodes.

1.2.1 Spring 1995: Upgrading the Computational Capability of the UIUC Group

In the first few months of this grant, in early 1995, a significant upgrade of the groups computational capability was achieved through the purchase of an SGI Power Challenge Server with 1 Gbyte of RAM (machine name Messiah). With the purchase of this machine, Stewart no longer needed to write separate proposals to the NSF supercomputing centers to get adequate computational cycles to carry out the research on the Directorates projects. The turnaround time on computational runs in the group dropped dramatically.

Because of the need to validate and to test DSD algorithms, the hydrocodes (DOE) MESA and (AF) EPIC were ported to the SGI Power Challenge. Both codes were chosen as target hydrocodes for the installment

of the DSD wave tracker (DKAPPA2D). Changes to program burn algorithms motivated by DSD-based analysis were identified through collaboration between Stewart and John Bdzil of Los Alamos National Laboratory (LANL).

1.2.2 Spring 1995: Design of AXS a New High Order Reactive Flow Code

In order to carry out validation studies of DSD and comparison with Direct Numerical Simulation (DNS) of reactive flow, it was deemed essential to write a new hydrocode that employed high order methods with 1990s algorithms. Previous attempts to measure detonation shock dynamics of a DNS in converging and diverging wedge geometries had been carried out by Tariq Aslam (a UIUC graduate student supported by this grant), Bdzil and Stewart with the use of (DOE/LANL) CAVEAT and MESA. Low accuracy measurements of the relation between the normal shock velocity, D_n and the shock curvature, κ were had been made with MESA. But an inherent difficulty was that the measurement of the shock curvature, the shock velocity and the shock acceleration required construction of derivatives of the motion of the shock surface and lab codes like, MESA, CAVEAT and EPIC did not have high accuracy algorithms.

In April of 1995 the new code, named AXS was designed in a collaboration between Stewart and his two students, Aslam and Xu. AXS used ENO-schemes that were 4th and 5th order spatially accurate. The work was documented in [6] and AXS was delivered in 1998 to Eglin engineer Michael Nixon. Two versions were written corresponding to the two students. Aslams version implemented reactive flow for an ideal equation of state, but importantly Xus implementation was for nonideal EOS. The second version of AXS was used to compute deflagration to detonation transition in porous and the nonideal version of AXS implemented a Glaister Riemann solver. This work was documented in [3]. The details of the algorithms can also be found in Xu's thesis, [17].

Also a paper on the level set implementation of DSD was completed during this period in the grant and it was later published in the Journal of Computational Physics, [2]. The level set code used for this paper was DKAPPA2D, written by Tariq Aslam as part of his PhD. thesis, [16].

1.2.3 Summer of 1995: Installation of the DSD Wave Tracker into EPIC Begins

In the summer of 1995, Stewart, Aslam and Directorate engineer Michael Nixon started the process of installing the DSD - wave tracker, DKAPPA2D into the Eglin-based code EPIC. A similar installation for MESA had already been carried out in collaboration with John Bdzil and colleagues at LANL, again with the use of DKAPPA2D. In addition a simple DSD program burn algorithm that had been devised by Stewart and Bdzil was implemented for the polytropic product EOS. The June of 1997 release of EPIC97 contained the DSD wavetracker in the form installed by Nixon.

1.2.4 Summer of 1995: Beginnings of NONIDK and DSD Characterization of Non-ideal Explosives

In the summer of 1995, Stewart worked out the basic formulation of the simplest DSD theory for a non-ideal explosive and sketched out a rough numerical treatment to solve the nonlinear eigenvalue problem for the $D_n - \kappa$ response. Later this effort resulted in the writing of NONIDK a code that generates the $D_n - \kappa$ response curve given a general non-ideal EOS and reaction rate law model. This early work was documented in [9].

1.2.5 Summer of 1995: Stewart and Ruderman Formulate an Approach to Modeling the Mechanical Ignition of Energetic Materials

In the summer of 1995, while visiting Eglin AFB, Stewart and graduate student Ruderman reviewed some of the approaches being used by Directorate engineers to understand and analyze Taylor Anvil impact experiments, being carried out at the AWEFT to characterize explosive damage and ignition. A conclusion was drawn that the state of modeling justified the effort to construct a new first principles continuum model. The explosive HMX was picked as a target material for the new modeling effort since thermomechanical data for HMX is relatively abundant. However, the modeling approach to be devised was to be general. It was decided that in order to properly described the ignition events in the AWEFT shear and impact experiments, that the phase transformations from solid to liquid and liquid to gas and subsequent gaseous combustion all needed to be included. If possible the physics of these disparate processes should be combined into one self-consistent continuum model.

Ruderman started collecting information on the kinetics and properties and phase transformations, particularly melting behavior of HMX. Later that fall of 95 and in the spring of 1996 Stewart and Ruderman began a collaboration with a UIUC TAM Professor Eliot Fried, to construct a phase-field continuum modeling of energetic materials. The model was designed to be thermodynamically consistent in three dimensions. The model has an order parameter as a field variable that is used to describe the material as a solid, liquid and gas. Also an independent reaction progress variable was introduced.

1.2.6 Fall 1995 through Spring 1996: Validation of DSD through Direct Comparison with DNS via AXS

In his thesis Aslam [16] demonstrated conclusively that one could do numerical experiments on detonation flows for a number of different experiments in different geometries, (converging channel wedge, expanding channel, and circular arc) and make direct measurement of the detonation dynamics. From the experimental records of the diffraction and convergence experiments it was shown that one could successfully construct consistent correlations that describe such independent experiments. From measurement of the shock dynamics observed in numerical experiments one was able construct a relationship between the shock acceleration, $\dot{D}_n$, the normal shock velocity D_n, and the shock curvature, κ relation without recourse to any theory. One could then independently solve the DSD-like evolution equations obtained from these measurements and compare the shock locations of the DSD-like prediction and the DNS.

The comparisons were found to be excellent across a huge range of detonation velocities, curvature and shock acceleration. The quality of the predictions and the fact that this very different methodology, much more akin to pure experimental work, achieved such good results was startling. This work also indicated the extreme importance of retaining the shock acceleration term $\dot{D}_n$ in both theory and computation as its inclusion made dramatic improvements in the quality of the DSD wave front predictions. In 1999 the paper, T. Aslam and D. S. Stewart, "Detonation shock dynamics and comparison with direct numerical simulation", appeared in Combustion Theory and Modeling, [12].

1.2.7 Summer of 1996: The Second AFOSR Grant, F49620-96-1-0260 Starts

In June of 1996, a second AFOSR Grant, F49620-96-1-0260 funded by Dr. Arje Nachman, or AFOSR Physical Mathematics Directorate, entitled "Analytical Investigations on Detonation Theory and Mechanical Ignition of Condensed Explosives" started. The topical coverage of the grant was designed to augment and complement the research goals of this grant, funded by the Directorate. The AFOSR grant provided funds for the Salary of Dr. Mark Short as a Research Associate. Dr. Short published a number of papers with Stewart on the stability of detonation, [4], [10], [13]. Computing resources and travel expenses were made available from this grant to support Dr. Short. Dr. Short visited Eglin AFB in the summer of 1997 and 1998 and began to interact with engineers at the AWEFT facility on issue associated with ignition of energetic materials.

1.2.8 Summer of 1997: Formulation of DSD - Cut, Explosive System's Detonation Shock Pressure Maps

A visit to Eglin AFB, in the Summer of 1997 by Stewart witnessed a number of important developments for enhanced DSD-design. In particular, in response to Directorate research on adaptable warheads, there was a discussion about using DSD in new ways and taking more advantage of the codes previously written. Stewart proposed a new engineering methodology, subsequently dubbed DSD-cut to distinguish it from the different use of DSD that was implemented in EPIC and MESA, subsequently named DSD-push.

The object of DSD-cut was to use DSD-computed estimates of the reaction zone structure of nonideal explosives to compute the peak detonation shock pressures and the reaction zone profiles generated by detonation prior to the impact on a metal target. Specifically the focus was on cutting metals. This work was deemed particularly relevant for explosives (typical of explosives used in insensitive munitions) with reaction zones that may be a long as 1/3 the thickness of the metal target plate.

The engineering strategy and a list of procedures and codes needed to carry out the DSD-engineering design calculations was outlined later in a TAM technical report no 869, " Detonation Shock Dynamics: Application for precision cutting of metal with detonation waves", [7]. Importantly a very simple concept of mapping the detonation shock pressure in the interior of an explosive is elucidated. Shock pressure maps allows a designer

immediate feedback on the placement of detonator points via the consistent use of the DKAPPA2D and DKAPPA3D class of codes. NOIDK provided a means to generate a new $D_n - \kappa$ relations for an explosive used in a design.

Figures 1. 2. and 3. show an expample of the DSD-based detonation shock pressure maps computed in the interior of an simple shaped charge geometry, taken from [7].

1.2.9 Summer 1997: Ehancements to NONIDK to Include Shock Acceleration Effects

During the summer of 1997, Stewart and Nixon worked to make NONIDK platform independent. It was necessary to replace the numerical integration subroutine in NONIDK so that it could run on Eglin platforms. More importantly Stewart added shock acceleration effects into a formulation of DSD theory that could be used for condensed explosives described by a nonideal EOS. This work led to a wholly new DSD - characterization code dubbed NONIDK+PLUS (to be distinguished from the earlier NONIDK).

However at about the same time, the simple (interpolated gas-solid) EOS treatments used to represent the reactive equation of state (an interpolated gas-solid EOS used in the first versions of NONIDK) became suspect. It was found that certain Hugoniots crossed and hence a new effort on obtaining better EOS models was deemed as essential in order to accurately model explosives.

1.2.10 Fall 1997: The Start of the Davis EOS Model

In November of 1997, W. C. Davis visited UIUC specifically to help with enhancing the reactive EOS. This was an important effort since the continued work on DSD - characterization of non-ideal explosives depended on making improvements to the EOS models. The advantage of the Davis/UIUC EOS is that the EOS forms used are based on explicit functional forms that could be used directly in NONIDK and NONIDK+PLUS. The most recent version of this combined EOS improvements and shock acceleration effects was documented in [14].

1.2.11 Spring 1998: DSD Literature Search, Invited Topical Review on DSD written

In the Spring of 1998 a substantial effort was made by Stewart to carry out a comprehensive literature review on shock dynamics and in preparation of

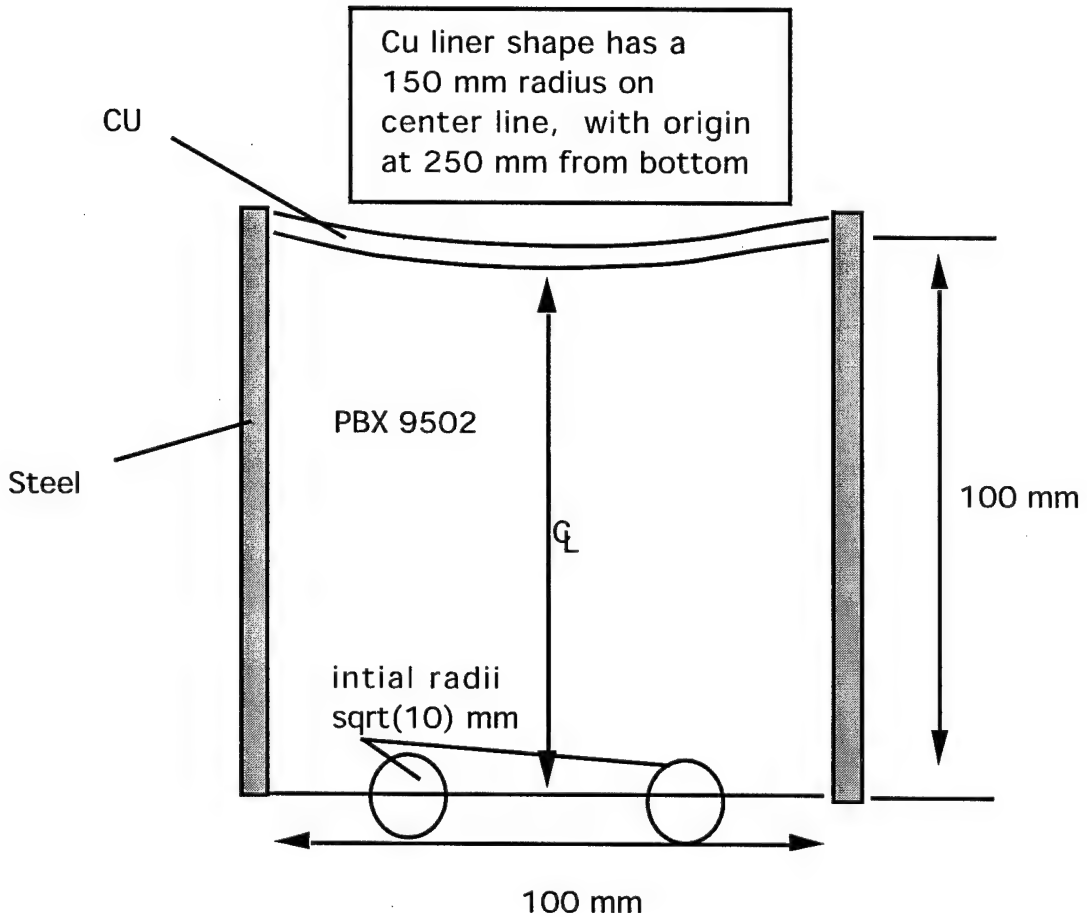

Figure 1: Design sketch for the worked example in the report [7]. The explosive is PBX9502, the side liners are steel and the top cup liner is copper. The dimensions are marked as shown.

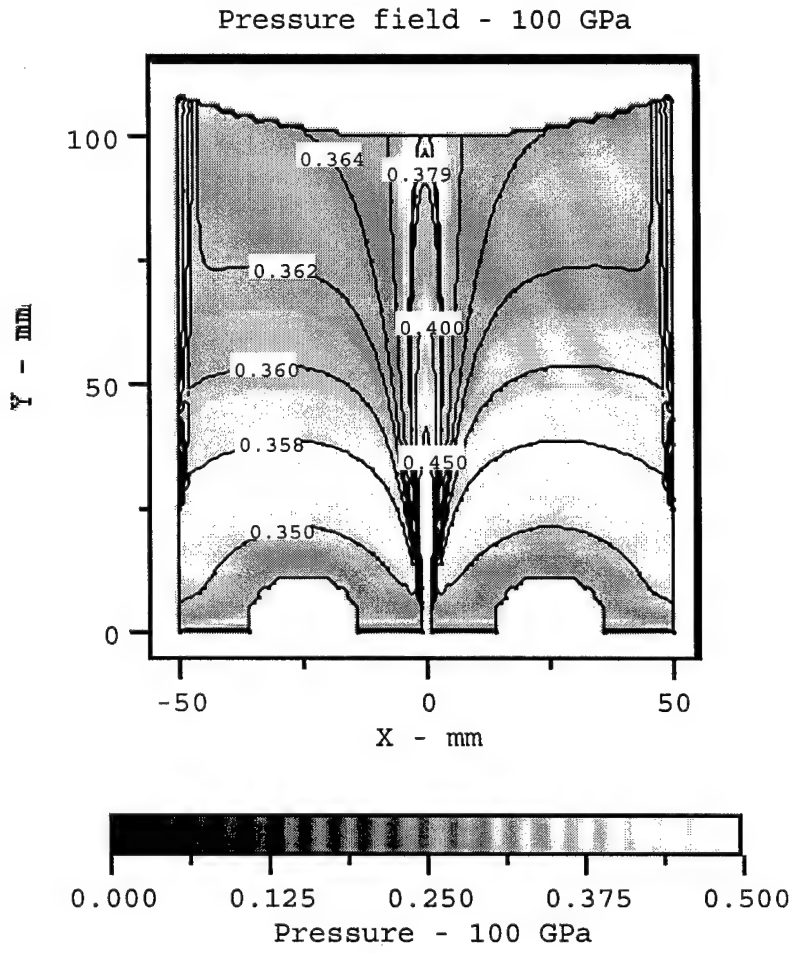

Figure 2: Grey-scale and line contour plot of the detonation shock pressure map for one detonator placement from [7].

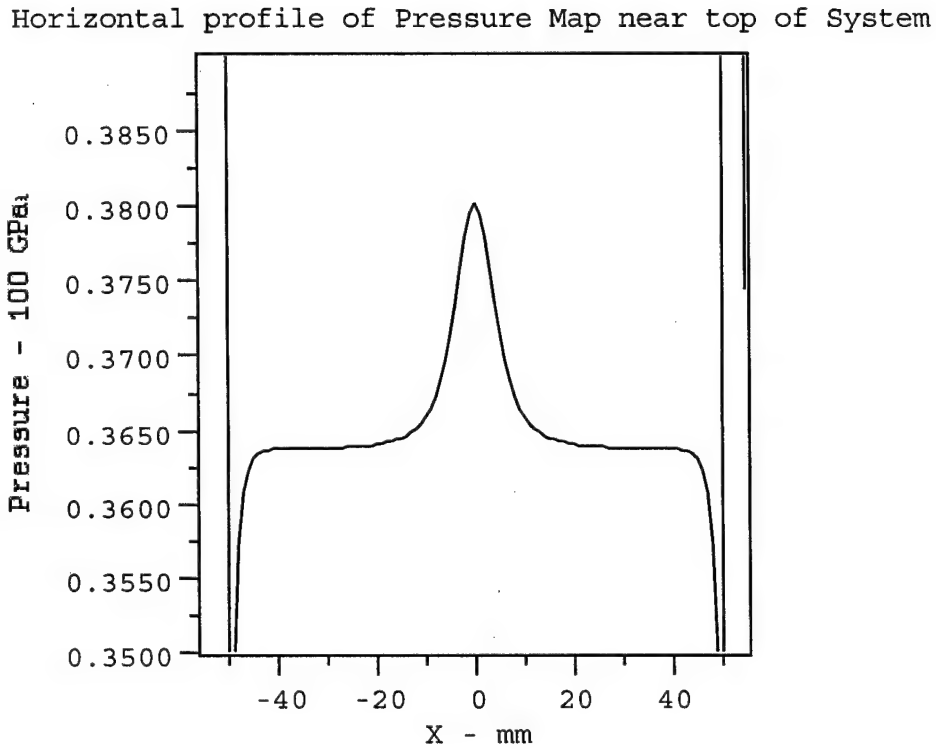

Figure 3: Horizontal profile of pressure mape near the top of the system for the first design.

book on detonation theory. An invited topical review was written for the Proceedings of the Combustion Institute, entitled, " The shock dynamics of multi-dimensional condensed and gas phase detonations", [11].

1.2.12 Spring 1998 - Summer 1998: Design of GIBBS1D by Ruderman and Stewart

In the early Spring of 1998 Stewart and Ruderman outlined the design of a new code specifically designed to solve the uni-directional motions of RSF-model. This code infrastructure was planned to solve one-dimensional, time-dependent PDEs that could handle the multi-scale physics of the phase transitions and the ignition events in the HMX model. The code suite was dubbed GIBBS1D.

It was also decided to use a simplified treatment of the material boundary where the displacement could be input. It was also decided to use ENO schemes and to adopt some of the same numerical strategies found in AXS. Ruderman began the code development with extensive testing and code validation. A copy of Ruderman's computer program used to simulation phase transition, (called GIBBS1D) was forwarded to Eglin engineers Michael Nixon and K. Vanden. This work was recorded in "Thermomechanical Modeling of Energetic Materials", [15] and was presented at the 10th Detonation Symposium in Snowmass CO in August 1998. A more detailed version of the work can be found in Ruderman's thesis, [19]. A substantial revision of this work is was being prepared for publication with current UIUC graduate student Jack Yoh.

1.2.13 Fall 1998: Preliminary DSD-Characterization of PBXN9 with NONIDK+PLUS

In the Fall of 1998, the Davis EOS was implemented in NONIDK+PLUS. A preliminary characterization of PBXN9 was carried out and rate law was modified so that the DSD, $D_n - \kappa$ curve for zero shock acceleration matched experimental data of L. Hull of LANL. Estimates of the shock acceleration behavior (contours of constant $\dot{D}_n$) for PBXN9 were generated automatically from NONIDK+PLUS. This preliminary DSD characterization of PBXN9 was reported to Directorate personnel in a March 1999 briefing at UIUC. The work is also recorded in [14].

1.2.14 Winter - Spring 1999: Simplified Derivation of the Theory of DSD

While working on draft introductory chapters of the book, Stewart sought to simplify the presentation of the DSD theory. In one of the drafts Stewart used the new formulation originally developed in the topical review paper, [11] to re-calculate the $\dot{D}_n - D_n - \kappa$ relation first given in [8]. With Yaos help, the new presentation is simpler and contains all the previous results. More importantly it generates new and simpler analytic formulas for the ideal EOS case. The ideal EOS case is an important test case and has been used to validate NONIDK+PLUS. The new asymptotics are also compared favorably against the numerical experiments of Aslam and Stewart found in [12]. One now has asymptotics, a general numerical treatment and direct numerical simulation all in agreement.

1.2.15 Spring 1999: Nineteen Point Detonation Array Simulations

In April 1999, Stewart visited Directorate personnel at Eglin AFB at AWEFT. After consultation with Dr. Joseph Foster, and Dr. David Lambert, a 3-dimensional DSD wave tracker simulation was run at UIUC for a 19 pt hexagonal pattern array of detonators, for the explosive PBXN9 simulant, inside a metal cylinder The tools that were used are DKAPPA3D and NONIDK+PLUS and the design logic discussed in [7]. The $\dot{D}_n = 0$ curve is used as the $D_n - \kappa$ relation for the explosive. A version of DKAPPA3D that was set-up to carry out the 19 point detonator array was transferred to Eglin engineer Michael Nixon. Figure 4. shows breakout time one millimeter from the top surface of a 19 point detonator system. A corresponding detonation shock pressure map of the top surface at break out is easily computed (not shown). The computations were done with DKAPPA3D, by Stewart and Yao in collaboration with Eglin, AWEFT egineers David Lambert and Joseph Foster. The $D_n - \kappa$ relation used was for a simulant of PBXN9.

2 Archival papers, Ph.D. theses and Reports

Below we list the most important papers, reports and Ph.D. theses that benefited wholly or in part from the resources of this grant. The entries appear in more or less chronological order and the reference number corresponds to the text of the preceding section. An abstract or summary of each entry is

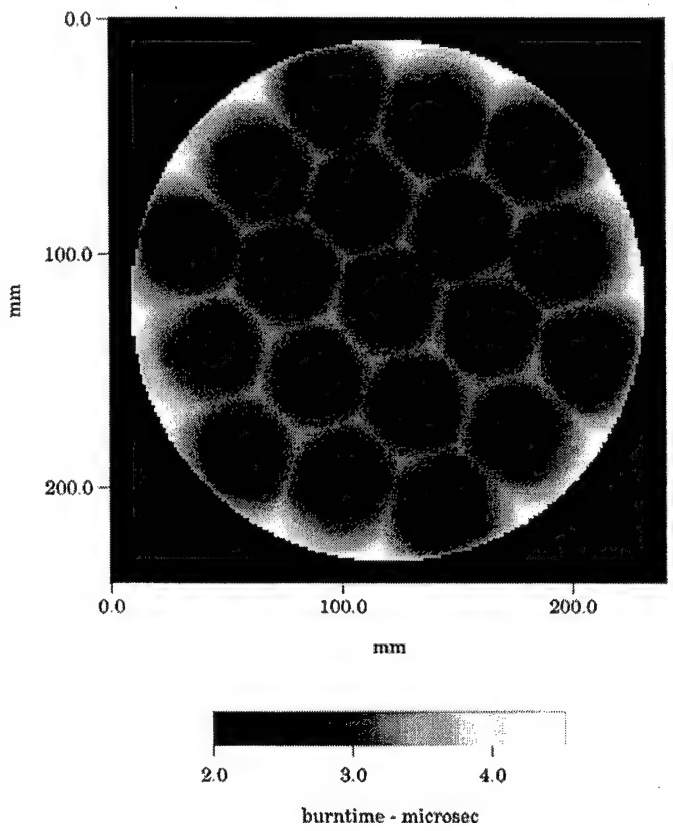

Figure 4: Map of the arrival time of a 19 point detonator system computed with DKAPPA3D for a PBXN9 explosive simulant, May 1999. The arrival time map corresponds to the cut pattern of a top metal plate induced by detonation in the explosive initiated by the 19 point array.

included to summarize the research findings in more detail.

References

2.1 Archival Papers and Technical Reports

[1] Yao, J. and Stewart, D. S. On the dynamics of multi-dimensional detonation. Journal of Fluid Mechanics 309, 225-275 (1996).

Abstract. We outline an asymptotic theory for the dynamics of detonation when the radius curvature of the detonation shock is large compared to the one-dimensional steady, Chapman-Jouguet (CJ), detonation reaction-zone thickness. The theory includes the limits of near-CJ detonation, and when the normal detonation velocity is significantly below its CJ-value. The curvature of the detonation can also be of either sign corresponding to both diverging and converging geometries. In particular, we derive an intrinsic, partial differential equation (PDE) for the motion of the shock surface, that is hyperbolic in character, and is a relation between the normal detonation shock velocity, shock curvature and the normal acceleration of the shock along its normal. The derivation includes consideration of additional time-dependence in the slowly-varying reaction-zone than that considered in previous works. A simpler version of the shock evolution equation is derived in the limit of large-activation energy. Illustrative examples of numerical solutions to hyperbolic evolution equations are presented.

[2] Aslam, T., Bdzil, J. B. and Stewart, D. S. Level-set methods applied to modeling detonation shock dynamics. Journal of Computational Physics 126, pp. 390-409 (1996).

Abstract. We give an extension of the level set formulation of Osher and Sethian, which describes the dynamics of surfaces that propagate under the influence of their own curvature. We consider an extension of the original algorithms for finite domains that includes boundary conditions. We discuss this extension in the context of a specific application that comes from the theory of detonation shock dynamics (DSD). We give an outline of the theory of DSD which includes the formulation of the boundary conditions that comprise the engineering model. We give the formulation of the level set method, as applied to our application with finite boundary conditions. We develop a numerical method to implement

arbitrarily complex 2D boundary condition and give a few representative calculations. We also discuss the dynamics of level curve motion and point out restrictions that arise when applying boundary conditions.

[3] Xu, S. and Stewart, D. S. Deflagration to detonation transition in porous energetic materials: A comparative model study. Journal of Engineering Mathematics, 31, 143-172 (1997).

Abstract. A numerical study of deflagration to detonation transition (DDT) in porous HMX is carried out. Three reactive-flow models varying from single phase to three phase formulation are chosen for the study. The GISPA model is a single-phase model and the BKS model is a simplified two-phase, gas and solid phase model. The SVG model is a three-phase model, which is based on evolution of solid, gas and void. The modeling assumptions made in construction of the SVG model are presented with a brief description of the other two models. In addition to hydrodynamic modeling, a new reaction-kinetics model, or rate law, is presented to model energy release. The rate law accounts for autocatalytic decomposition of HMX and pressure dependent shock to detonation transition kinetics. The model results are compared in detail against the DDT events observed in physical experiments. Numerical simulation of inert compaction waves and DDT is carried out for parameters suitable for powdered HMX. The simulation shows that all three models can effectively predict: (a) the formation of a secondary compaction wave and a high-density plug, (b) initiation of the transition to detonation in front of the plug and (c) the survival of the plug residual after the detonation. The SVG model compares the best against the measurable data of the physical experiment and is also computationally efficient and well-posed. Therefore it is a good candidate for multi-dimensional DDT calculations.

[4] Short, M. and Stewart, D. S. Low-frequency, two-dimensional, linear instability of plane detonation. Journal of Fluid Mechanics, 340, pp. 249-295, (1997).

Abstract. An analytical dispersion relation describing the linear stability of a plane detonation wave to low-frequency two-dimensional disturbances with arbitrary wavenumbers is derived using a normal mode approach and a combination of high activation energy and Newtonian limit asymptotics, where the ratio of specific heats tends to one. The reaction chemistry is characterized by one-step Arrhenius kinetics. The analysis assumes large activation energy in the plane steady-state detonation

wave and a characteristic linear disturbance wavelength, which is longer than the fire-zone thickness. Newtonian limit asymptotics are employed to obtain a complete analytical description of the disturbance behavior in the induction zone of the detonation wave. The analytical dispersion relation that is derived depends on the activation energy and exhibits favorable agreement with numerical solutions of the full linear stability problem for low-frequency one- and two-dimensional disturbances, even when the activation energy is only moderate. Moreover, the dispersion relation retains vitally important characteristics of the full problem such as the one-dimensional stability of the detonation wave to low-frequency disturbances for decreasing activation energies or increasing overdrives. When two-dimensional oscillatory disturbances are considered, the analytical dispersion relation predicts a monotonic increase in the disturbances growth rate with increasing wavenumber, until a maximum growth rate is reached at a finite wavenumber. Subsequently the growth rate decays with further increases in wavenumber until the detonation becomes stable to the two-dimensional disturbance. In addition, through a new detailed analysis of the behavior of the perturbations near the fire front, the present analysis is found to be equally valid for detonation waves traveling at the Chapman-Jouguet velocity and for detonation waves which are overdriven. It is found that in contrast to the standard imposition of a radiation or piston condition on acoustic disturbances in the equilibrium zone for overdriven waves, a compatibility condition on the perturbation jump conditions across the fire zone must be satisfied for detonation waves propagating at the Chapman-Jouguet detonation velocity. An insight into the physical mechanisms of the one- and two-dimensional linear instability is also gained, and is found to involve an intricate coupling of acoustic and entropy wave propagation within the detonation wave.

[5] Stewart, D. S., Aslam, T.D. and Yao, J. On the evolution of detonation cells. Proceedings of the 26th International Symposium on Combustion, pp. 2981-2989 (1997).

Abstract. A detonation shock-evolution equation that predicts both pulsating and cellular detonation has been derived in the limit of near-Chapman-Jouguet detonation, weak curvature, slow temporal variation and large activation energy with a newly applied technique of the method of successive approximation. The evolution equation describes a wave-hierarchy that is consistent with the linear stability theory of the evolution equation. We define the parameter regime for which the equation

applies. The transverse wave instability, as indicated from analysis, leads to cellular detonation. Triple-point tracks correspond to shock-shock intersections of the dynamics solution of smooth portions of the front. The dynamics of the cellular solutions are consistent with the notion that the power of the detonation front is derived from the normal reaction zone and the triple points are generated as the interaction of the independently propagating fronts and the consequent shock-shock intersections, not as the centers of blast waves. Explicit criteria for prediction of cell widths and cell aspect ratios are given.

[6] Xu, S., Aslam, T. and Stewart, D. S. High-resolution numerical simulation of ideal and non-ideal compressible reaction flow with embedded internal boundaries, 1, No. 1., 113-142, (1997).

Abstract. This paper explains the methodology used to develop a high-resolution, multi-dimensional Euler solver that is capable of handling non-ideal equation of state and stiff chemical source terms. We have developed a pointwise implementation that has computational advantages for our intended application, as opposed to a finite volume implementation. Our solver allows for the placement of internal reflective boundaries and the standard inflow and outflow and reflective boundaries at the edge of the domain. We discuss the spatial discretization and the temporal integration schemes, upwinding and flux splitting and the combined use of the Lax-Friedrichs and Roe schemes to solve for the required fluxes. A complete description of the pointwise internal boundary method is given. An overall summary of a representative code structure is given. We provide details on the verification of our integrated set of algorithms that resulted in an application code. We demonstrate the order of convergence for test problems. Two example applications from measurement of detonation shock dynamics and deflagration to detonation transition in porous energetic materials are presented.

[7] Stewart, D. S, Detonation shock dynamics: Application for precision cutting of metal with detonation waves, TAM Report, No. 869, UILU-ENG-97-6030, October 1997.

Abstract. This technical report starts with an introduction about the engineering use of detonation shock dynamics and its advantages. Next there is a review of the relevant basics of DSD-theory that include the reduced governing equations, the Rankine-Hugoniot relations and CJ-state, the formulation of the basic eigenvalue problem that is used to relate the

normal detonation velocity and the shock curvature and representative results for PBX9502. The next section explains how to make shock pressure maps in the interior of an explosive system. First the DSD wave tracker is run on the explosive domain, then the shock pressure is computed. Comments are made on the interpretation of the maps for design purposes.

[8] Buckmaster, J., Short M. and Stewart, D. S. The use of activation energy asymptotics in detonation theory, with Comment on "Multidimensional stability analysis of overdriven gaseous detonation, Phys. Fluids 9, 3764, Physics of Fluids, 10, 3027-3030 (1998).

Abstract. A powerful defense is given for the use of activation energy asymptotics in opposition to erroneous and misleading work carried out by Clavin and Williams.

[9] Stewart, D. S. and Yao, J. The normal shock velocity-curvature relationship for materials with non-ideal equation of state and multiple turning points. Combustion, 113, 224-235 (1998).

Abstract. We present a model and simple to implement numerical procedure that obtains the normal detonation shock velocity curvature relationships for an explosive material with non-ideal equation of state and an arbitrary reaction rate law. In addition we illustrate numerically (for a non-ideal equation of state) and analytically (for an ideal equation of state with a large activation energy rate law) that for sufficient rate-state -sensitive explosives, the response curve can have two turning points such that the curve has a Z-shape. The top branch of the Z response curve has been previously been associated with detonation extinction at a critical curvature. The bottom branch can be possibly associated with low velocity detonation and rapid change from low order detonation to high order.

[10] Short, M. and Stewart, D.S. Cellular detonation stability: A normal mode linear analysis. Journal of Fluid Mechanics, 368, 229-262 (1998).

Abstract. A detailed investigation of the hydrodynamic stability of a steady, one-dimensional detonation to transverse linear disturbances in an ideal gas undergoing an irreversible, unimolecular reaction with an Arrhenius rate constant is conducted via a normal-mode analysis. The method of solution is an iterative shooting method, which integrates between the

detonation shock and reaction equilibrium point. Variations in the disturbance growth rates and frequencies with transverse wavenumber, together with two-dimensional neutral stability curves and boundaries for all unstable low- and high-frequency modes are obtained for varying detonation bifurcation parameters. These include the detonation overdrive, chemical heat release and reaction activation energy. Spatial perturbation eigenfunction behavior and phase and group velocities are also obtained for selected sets of unstable modes. Results are presented for both Chapman-Jouguet and overdriven detonation velocities. Comparisons between the earlier pointwise determination of stability and interpolated neutral stability boundaries obtained by Erpenbeck are made. Possible physical mechanisms which govern the wavenumber selection underlying the initial onset of either regular or irregular cell patterns are also discussed.

[11] Stewart, D. S. The shock dynamics of multi-dimensional condensed and gas phase detonations. Proceedings of the 27th International Symposium on Combustion, pp. 2189-2205 (1998)

Abstract. Detonations are comprised of broad detonation shock supported by thin reaction zone. Approximation base on weak shock curvature measured on the inverse reaction zone scale, and quasi-steady flow, measured on the particle passage time through the reaction zone can be used to simplify the mathematical description of detonations that are governed by the gasdynamic equations for a reacting flow. When the detonation reaction zone contains a sonic locus it is possible to derive intrinsic (coordinate independent) partial differential equation for the lead detonation shock's motion in terns of the normal detonation shock velocity, the shock curvature and higher normal time derivatives. We refer to this collection of theory and supporting experimental results as Detonation Shock Dynamics after Whitham's Geometrical Shock Dynamics. The reduce detonation dynamics is based on the concept of an eigenvalue (sonic) detonation, an idea that goes back to the original investigations in the 1940's. We present a review of the theoretical and experimental developments and attempt to update Fickett and Davis' discussion of work prior to 1980. We give examples of the theory and applications which include: i) weakly-curved, quasi-steady, near-CJ detonation ii) critical detonation curvature iii) quasi-steady extinction and ignition (and low velocity detonation) iv) shock acceleration effects and v) cellular and pulsating detonation in gases. We also review the engineering method of Detonation Shock Dynamics as it is applied to explosive systems.

[12] Aslam, T.D. and Stewart, D.S. Detonation shock dynamics and comparisons with direct numerical simulation, Combustion Theory and Modeling, 3, 77-101 (1999)

Abstract. Comparisons between direct numerical simulation (DNS) of detonation and detonation shock dynamics (DSD) is made. The theory of DSD defines the motion of the detonation shock in terms of the intrinsic geometry of the shock surface, in particular for condensed phase explosives the shock nomrl velotiey, D_n, the normal acceleration, $\dot{D}_n$ and the total curavture, κ. In particular, the properties of three intrinsic front evolution laws are studied and compared. This are (i) constant speed detonation (Huygens's construction), (ii) curvature-dependent speed propagation ($D_n - \kappa$ - relation) and (iii) curvature speed-dependent acceleration ($\dot{D}_n - D_n - \kappa$ relation). We show that it is possible to measure shock dynamics directly from simulation of the reactive Euler equations and that subsequent numerical solution of the intrinsic partial differetial equation for the shock motion (e.g. a $\dot{D}_n - D_n - \kappa$ relation) reproduces the computed shock motion with high precision.

[13] Short, M. and Stewart, D. S. The multi-dimensional stability of weak heat release detonations. J. Fluid Mech., s382, 109-135 (1999).

Abstract. The stability of an overdriven planar detonation wave is examined for a one-step Arrhenius reaction model with an order one post-shock temperature-scaled activation energy in the limit of a small post-shock temperature-scaled heat release. The ratio of specific heats, is taken to be close to one. Under these assumptions, which cover a wide range of realistic physical situations, the steady detonation structure can be evaluated explicitly, with the reactant mass fraction described by an exponentially decaying function. The analytical representation of the steady structure allows a normal-mode description of the stability behavior to be obtained via a two-term asymptotic expansion in the heat-release. The resulting dispersion relation predicts that for a finite overdrive the detonation is always stable to two-dimensional disturbances. For large overdrives, the identification of regimes of stability or instability is found to depend on a choice of distinguished limit between the heat release and the detonation propagation Mach number. Regimes of instability are found to be characterized by the presence of a single unstable oscillatory mode over a finite range of wavenumbers.

[14] Stewart, D. S. and Yao, J., Computation of shock acceleration effects on detonation shock dynamics for explosives described by general equation of state, to appear Proceedings of the 28th International Symposium on Combustion.

Abstract. The inclusion of detonation shock acceleration effects leads to an extended theory of Detonation Shock Dynamics (DSD). The shock motion is described by an intrinsic partial differential equation specified in terms of the normal shock velocity, D_n, the normal shock acceleration $\dot{D}_n$ and the curvature κ. Earlier developments were based on analytical (asymptotic) calculations and carried out for the polytropic equation of state that made detailed analysis tractable. But the demands of quantitative accuracy for engineering design require that real equation of state constitutive forms be used with more functional complexity. In this paper we present a numerical approach that can be used to compute the $\dot{D}_n, D_n, \kappa$-relation for general EOS and rate law forms.

[15] Ruderman, G., Stewart D. S. and Fried, E. ". Modeling the Mechanical Ignition Energetic Materials, Proceedings of the 11th (International) Symposium on Detonation, Office of Naval Research, pp 554-561 (2000)

Abstract. A new theory of continuum thermomechanics involving microforces, or forces which drive the evolution of the microstructure in a material, is applied to the modeling of energetic materials, specifically, HMX. Using this theory, a set of partial differential equation are derived in a consistent thermodynamic framework which models HMX as a nonlinearly viscoelastic solid capable of undergoing phase transition to a viscous liquid and ideal gas, as well as a combustion process from unreacted HMX to reacted products. This system was then simplified to a set of one-dimensional model problems, which were solved numerically using advance computation techniques including essentially non-oscillatory (ENO) methods.

2.2 Phd. Theses Supported by the Grant

[16] Aslam, T. D., Investigations of Detonation Shock Dynamics, Ph. D. thesis, University of Illinios, 1996, Theoretical and Applied Mechanics, thesis advisor D. S. Stewart

Abstract. A detonation is a combustion driven shock wave. Typically, a detonation will consist of an inert shock followed by a region of chem-

ical reaction referred to as the reaction zone. Detonations have a wide variety of engineering applications, from obvious military use to explosive welding, hard rock mining and materials processing. Detonations can occur in a variety of materials, including gases (such as premixed hydrogen and oxygen), liquids, and solid explosives. Of particular interest in detonation problems is the motion of the detonation shock. Changes to the reaction zone may cause large variations in the strength and speed of the detonation front, so it can not be ignored in modeling detonations. For typical explosives, the reaction zone may be thousands of times smaller than the engineering scale. This multi-scaled nature of detonation can pose problems when trying to predict the motion of the detonation front.

Detonation shock dynamics is an asymptotic theory whose key result is an intrinsic partial differential equation for the dynamics of the detonation shock front. It will be demonstrated that the theory can predict several aspects of unsteady multi-dimensional detonation accurately. Three intrinsic relations will be examined and compared with direct numerical simulation. Their relevance to modeling detnation dynamics will also be given. Numrical methods based on level-set ideas, will be given for propagating multi-dimensional detonation fronts in arbitrarily complex geometries.

[17] Xu, Shaojie, Modeling and numerical simulation of deflagration to detonation transition in porous energetic materials, Ph. D. thesis, University of Illinios, 1996, Theoretical and Applied Mechanics, thesis advisor D. S. Stewart

Abstract. An understanding of the deflagration-to-detonation transition (DDT) in porous energetic materials is important to various engineering applications. Safety issues of explosives, specifically the prevention of accidental detonation is damaged explosive, is one example. The transition process is complex in nature and involves both subsonic and supersonic phenomena such as compaction and detonation respectively. The presence of multiple time and length scales makes the study of DDT challenging and interesting. Modern computational technology has made a great impact on the study. Numerical simulation becomes an important a necessary means to carry out the study, especially for problems arising from engineering applications. Two topics related to multi-dimensional simulation of DDT in energetic materials are presented in this work.

The objective of the first part is to develop a model that has a relatively simple mathematical structure. Two-phase mixture theory has been used

over the past two decades to describe DDT in porous energetic materials. Conservation laws of mass, momentum and energy are written independently for two materials, and the interactions between the phases are represented by source terms. Models constructed by the theory usually have complicated structures represented by a large set of governing equations and complex wave structures. Hence, it is difficult to resolve them numerically with the computational power available. Three simplified DDT models name Bdzil-Kapila-Stewart (BKS), solid-void-gas (SVG) and gas-interpolated solid Stewart Prasad Asay (GISPA), are considered in the current study; among them SVG and GISPA are newly developed. These models are base on a single velocity formulation and thus have fewer governing equations and simple wave structures. A comparative study is carried out based on the three models. The purpose of the study is to identify a minimum set of elements possessed by a model to make predictions consistent with experiments. The study shows that the SVG mode is the best among the three models over a wide range of experimental data.

In addition to model simplification, effort has been focused on chemical reaction kinetic modeling, which describes energy release during the reaction process. Previously used chemical kinetic models, or reaction-rate laws, are not adequate to predict detonation initiation. A new reaction rate law is developed which employs two different rate functions associated with slow and fast energy-release processes that have been observed in experiments. With the new rate law, the SVG and GISPA models are able to predict qualitatively and quantitatively all the events recorded in one-dimensional DDT tube experiments.

The second part of the study is devoted to the development of a high-quality numerical method, suitable for multi-dimensional direct numerical simulation of DDT with non -linear material on a complex geometry. The method is developed through an integration of contemporary shock-capturing methods. The new finite-difference scheme adopts the method-of-lines approach, which allows for independent temporal and spatial discretizations. The temporal integration uses a third-order Runge-Kutta method with the property of total variation diminishing (TVD), while the spatial integration employs a fourth-order essentially non-oscillatory (ENO) scheme. In order to implement the scheme for nonlinear material, a Roe's linearized Riemann solver is developed in two dimension for an equation of state that describe an HMX material To fulfill the needs of engineering applications, an internal boundary method is de-

veloped on a structured grid. The internal boundary algorithm allows a two-dimensional non-deformable body of arbitrary shape to be inserted in a flow field. A second-order reflective boundary condition is implement along the internal boundary. The new scheme, equipped with the internal boundary algorithm, provides great flexibility for numerical simulation of engineering problems with complex boundaries. A two-dimensional DDT simulation is carried out to simulate a blunt body impact on energetic materials. A bullet with a circular head is imbedded in a square body of HMX material and is subjected to an impulsive motion. The radius effect on transition to detonation is studied. A sharp body impact is also considered where the circular bullet head is replaced by a wedge.

[18] Yao, J. The dynamics of multi-dimensional detonation. Ph. D. thesis, University of Illinois, 1996, Theoretical and Applied Mechanics, thesis advisor D. S. Stewart

Abstract. An asymptotic theory is presented for the dynamics of detonation when the radius of curvature of the detonation shock is large compared with one-dimensional steady Chapman-Jouguet (CJ) detonation reaction-zone thickness. The analysis considers additional time-dependence in the slowly-varying reaction zone than that considered in previous works. The detonation is assumed to have a sonic point in the reaction-zone structure behind the shock, and is referred to as an eigenvalue detonation. A new iterative method is used to calculate the eigenvalue relation, which ultimately is expressed as an intrinsic partial differential equation (PDE) for the motion of the shock surface. Two cases are considered for an ideal equation of state. The first corresponds to a model of a condensed phase explosive, with model reaction-rate sensitivity, and the intrinsic shock surface PDE is a relation between the normal detonation shock velocity, D_n, the first normal time derivative of the normal shock velocity, $\dot{D}_n$, and the shock curvature κ. The second case corresponds to a gaseous explosive mixture, with the large reaction-rate sensitivity of Arrhenius kinetics, and the intrinsic shock surface PDE is a relation between the normal detonation shock velocity D_n, its first and second normal time derivatives $\dot{D}_n$, $\ddot{D}_n$, the shock curvature κ, and the first normal time derivative of the curvature $\dot{\kappa}$. For the second case, one obtains a one-dimensional theory of pulsation of plane CJ detonation and a theory that predicts the evolution of self-sustained cellular detonation. Versions of the theory include the limit of near-CJ denotation, and the limit in which the normal detonation velocity is significantly below

its CJ value. The curvature of the detonation can also be of either sign corresponding to either diverging or converging geometry.

The linear instability of a weakly curved slowly varying detonation wave is also investigated under the assumption of frozen curvature. The governing equations and the boundary conditions required to formulate the instability problem are derived. The steady $D_n - \kappa$ relation and the quasi-steady state of the weakly curved detonation have been obtained numerically. The eignvalues of the acoustic instability are calculated by a numerical shooting method.

[19] Ruderman, G. A., A Continuum Thermomechanical Model for Energetic Materials, Ph. D. thesis, University of Illinois, 1998, thesis advisor D. S. Stewart, TAM.

Abstract. Thermomechanical modeling of energetic materials, for example solid rock motor propellants and explosives, is a complex problem due to the large number of behaviors such a material may exhibit. Experiments have shown that these materials are nonlinearly viscoelastic, and may also experience plastic flow permanent deformation) phases changes (melting and vaporization processes), and combustion. In addition, these phenomena are often strongly coupled, making modeling very difficult. Compounding this difficulty further, reliable experimental data on the properties of these types of materials are quite scarce.

Applying advanced tools of continuum thermomechanics, we have developed a fully three-dimensional framework, which, in the most general form, is able to model all the mentioned behaviors of energetic materials. The concept of a balance of micro-forces, which drives changes in material microstructure, is employed to generate thermomechanically consistent equations of evolutions for combustion and phase transition.

The model is the simplified to a set of three model problems: the constant-volume thermal explosion, one-dimensional shear loading, and one-dimensional longitudinal loading. These model problems were solved numerically using essentially non-oscillatory and total variation diminishing methods. The solutions reveal extremely rich behavior, including complex wave phenomena, strain localization phenomena, and changes of material phase.

3 Faculty/Research Associates/Student Supported

- Tariq Asalm, supported as a research assistant, now a staff member at Los Alamos National Laboratory
- Shaojie Xu, partially supported as a research assistant, currently a research engineer on advanced computation for INTEL Corporation.
- Jin Yao, supported as a research assistant and one year as a PostDoctoral student, now with Orlando Technologies Incorporated, based in Ft. Walton Beach, Florida area.
- Mark Short, partial support as a research Associate and Visiting Assistant Prof. Now a tenure track Assistant Professor of Mechanics at UIUC.
- Gregory A. Ruderman, research assistant and USFAF Palace Knight. (Ruderman's travel expenses to Eglin AFB, were partially support by this grant). Ruderman graduated in the Fall of 1998, and returned to a position in the Rocket Motor Branch of the Propulsion Directorate and Edwards, AFB, California.
- Jack Yoh, research assistant who joined Stewart's group in 1998. Jack is currently working on multi-material simulations and ignitions studies in HMX.

DISTRIBUTION LIST
AFRL-MN-EG-TN-2001-7070

Defense Technical Information Center 8725 John J. Kingman Road, Ste 0944 Ft Belvoir, VA 22060-6218	1

EGLIN AFB OFFICES:

AFRL/MN CA-N	1
AFRL/MNOC-1 (STINFO Office)	1
AFRL/MNMW	3
AFRL/MNAC (Mr. Mike Nixon)	1